

Lattice QCD meets experiment in hadron physics

Christine Davies* and Peter Lepage†

**Dept. of Physics and Astronomy, University of Glasgow, Glasgow, G12 8QQ, UK*

†Laboratory for Elementary-Particle Physics, Cornell University, Ithaca, NY 14853, USA

Abstract. We review recent results in lattice QCD from numerical simulations that allow for a much more realistic QCD vacuum than has been possible before. Comparison with experiment for a variety of hadronic quantities gives agreement to within statistical and systematic errors of 3%. We discuss the implications of this for future calculations in lattice QCD, particularly those which will provide input for B factory experiments.

INTRODUCTION

QCD is a key component of the Standard Model of particle physics. It gives us a rich spectrum of bound states of quarks and gluons whose properties are predictable from QCD if we can solve the theory. QCD is strongly coupled in this regime, however, and we need the non-perturbative techniques of lattice QCD to do this from first principles.

Most (but not all) questions which lattice QCD can address require calculations with a precision of a few percent to answer them. These include the spectrum of hadrons, their internal structure and decay rates. In particular, the hunt for internal inconsistencies in the Standard Model which could lead to new physics requires calculations of hadronic weak matrix elements to 2-3% to match the experimental errors that will become possible.

Figure 1 shows the recent status of the combined experimental and theoretical efforts to pin down the vertex of the Cabibbo-Kobayashi-Maskawa unitarity triangle [1]. The different circular constraints on the vertex come from different decay rates of B and K mesons and are found by dividing experimental rates by theoretical results obtained in lattice QCD. The current constraints are strongly limited by current lattice QCD errors of around 20%.

Lattice QCD is hard and numerically very expensive. Recent progress [2] has at last made precision calculations look possible and we will concentrate on that work and its implications in this review.

LATTICE QCD CALCULATIONS

Lattice QCD calculations proceed by the discretisation of a 4-d box of space-time into a lattice. The QCD Lagrangian is then discretised onto that lattice. The spacing between the points of the lattice, a , is $\approx 0.1\text{fm}$ in current calculations and the length of a side of the box is $L \approx 3.0\text{fm}$. Thus our simulations can cover energy scales from $\approx 2\text{GeV}$ down

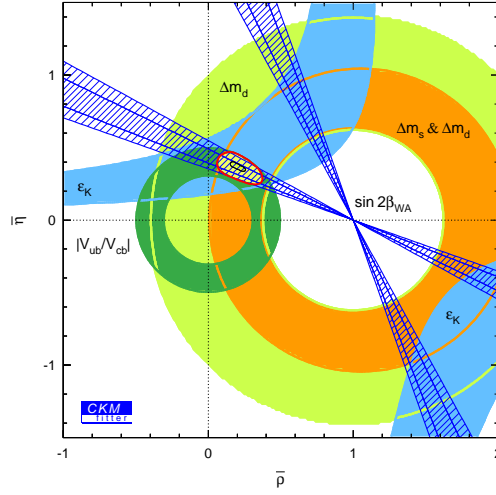


FIGURE 1. Recent constraints on the unitarity triangle from CKMfitter [1]

to ≈ 100 MeV.

The Feynman Path Integral is evaluated numerically in a two-stage process. In the first stage sets of gluon fields (‘configurations’) are created which are representative ‘vacuum snapshots’. In the second stage, quarks are allowed to propagate on these background gluon field and hadron correlators are calculated. The dependence of the correlators on lattice time is exponential. From the exponent the masses of hadrons of a particular J^{PC} can be extracted, and from the amplitude, simple matrix elements.

QCD as a theory has a number of unknown parameters, the overall dimensionful scale of QCD (\equiv the bare coupling constant) and the bare quark masses. To make predictions, these parameters must be fixed from experiment. In lattice QCD we do this by using one hadron mass for each parameter. The quantity which is equivalent to the overall scale of QCD on the lattice is the lattice spacing.

Lattice calculations are hard and time-consuming. Progress has occurred in the last thirty years through gains in computer power but also, often more importantly, through gains in calculational efficiency and physical understanding. One particular area which revolutionised the field from the mid-1980s was the understanding of the origin of discretisation errors and their removal by improving the lattice QCD Lagrangian. Discretisation errors appear whenever equations are discretised and solved numerically. They manifest themselves as a dependence of the physical result on the unphysical lattice spacing. In lattice QCD, as elsewhere, they are corrected by the adoption of a higher order discretisation scheme. The complication in a quantum field theory like QCD is the presence of radiative corrections to the coefficients in the higher order scheme which must be determined (using perturbation theory, for example [3]).

Physical understanding of heavy quark physics on the lattice has also made a huge difference to the feasibility of calculating matrix elements relevant to the B factory programme on the lattice. The use of non-relativistic effective theories requires the lattice to handle only scales appropriate to the physics of the non-relativistic bound states and not the (large) scale associated with the b quark mass. B physics is now one of the

areas where lattice QCD can make most impact.

One area which has remained problematic, but which this year's results have addressed successfully, is the handling of light quarks on the lattice. In particular the problem is that of how to include the dynamical (sea) $u/d/s$ quark pairs that appear as a result of energy fluctuations in the vacuum. We can safely ignore $b/c/t$ quarks in the vacuum because they are so heavy, but we know that light quark pairs have significant effects, for example in screening the running of the coupling constant and in generating Zweig-allowed decay modes for unstable mesons.

Because quarks are fermions, they cannot be simulated directly on the computer, but must be 'integrated out' of the Feynman Path Integral. This leaves an QCD Lagrangian in terms of gluon fields which includes $\ln(\det(M))$ where M is an enormous ($10^7 \times 10^7$) sparse matrix. The inclusion of dynamical quarks is then numerically very expensive, particularly as the quark mass is reduced towards the small values which we know the u and d quarks have.

Many calculations even today use the 'quenched approximation' in which the light quark pairs are ignored. Results then suffer from a systematic error of $\mathcal{O}(20\%)$. A serious problem with the quenched approximation is the lack of internal consistency which means that the results depend on the hadrons that were used to fix the parameters of QCD. This ambiguity plagues the lattice literature.

Other calculations have included 2 flavours of degenerate dynamical quarks, i.e. u and d , but with masses $10\text{-}20\times$ the physical ones. This approximation is better than the quenched approximation but large uncertainties remain because the s quark is omitted. Results must also be extrapolated to the physical u/d quark mass and chiral perturbation theory is a good tool for this. However, chiral perturbation theory only works well if the u/d quark mass is light enough and, for errors at the few percent level, this means less than $m_s/2$. This has been impossible to achieve in most calculations.

New results this year [2] have included u, d and s quarks in the vacuum, with light enough u/d masses to perform accurate chiral extrapolations. The results use a new discretisation of the quark action - the numerically fast improved staggered formalism. This formalism is well-matched to the supercomputing power of a few Tflops that is currently achievable.

Improved staggered quarks

The starting point for the staggered quark formalism is the naive discretisation of the Dirac quark action onto a lattice. This action has good features: chiral symmetry and discretisation errors that appear only as the square and higher powers of the lattice spacing. The naive discretisation suffers from the notorious doubling problem, however. A single quark species on the lattice gives rise to 16 quark species, or tastes, on a 4-d lattice. The additional tastes appear around the edges of the Brillouin zone, where $p \approx \pi/a$, as copies of a $p \approx 0$ quark. This would not be a problem if there were no interaction between the different tastes since the quark action would then fall apart into 16 different pieces in an appropriate basis and we could take $\det(M)^{(1/16)}$ in simulations to give the effect of 1 quark flavour.

There is interaction between the different tastes, however. It is mediated by highly virtual gluons, with momenta around π/a . A quark of one taste can absorb or emit such a high momentum gluon and turn into a quark of another taste. The effects of this taste-changing interaction are quite severe for the naive action, giving rise to large discretisation errors (even though formally of $\mathcal{O}(a^2)$) and large perturbative renormalisation factors, e.g. for the quark mass, when translating from the lattice scheme to the continuum. The degeneracy in mass of mesons made from quarks of different taste is lost. This is most noticeable for the pions because there is a light Goldstone boson.

Because the taste-changing interaction is a high momentum one it can be understood in lattice perturbation theory. In particular, the effects can be significantly improved by suppressing the coupling of quarks to gluons of momenta π/a in any direction. This is achieved by ‘smearing’ the gluon field in the action in a particular way [4, 5], and can be thought of as part of the standard Symanzik programme for systematically removing discretisation errors from lattice actions.

It is simple to ‘stagger’ the naive action and its improved variant to remove an exact degeneracy of a factor of 4 in tastes which arises from the spin degree of freedom. This results in an action with 4 doublers which can be simulated on the lattice using $\det(M)^{(1/4)}$ per flavour. It is very fast numerically because there is only one spin degree of freedom per site and the eigenvalues of M are well behaved. This is what has allowed the MILC collaboration to generate ensembles of configurations which include u , d , and s quarks in the vacuum with much more realistic masses than before [6].

Some worries remain about potential non-locality in the action as the result of taking the fourth root. However, this causes no problem in perturbative QCD where a simple power series in x is obtained for an action with $\det(M)^x$. Stringent non-perturbative tests are also then needed. Luckily these tests are possible in this formalism with present day computers because of its speed, and are exactly the calculations required to test (lattice) QCD. The results, shown in the next section, speak for themselves.

RECENT RESULTS

The MILC collaboration have made sets of ensembles of gluon field configurations which include 2 degenerate light dynamical quarks (u, d) and 1 heavier one (s) [6]. Taking the u and d masses the same makes the lattice calculation much faster and leads to negligible errors in isospin-averaged quantities. The dynamical s quark mass is chosen to be approximately correct based on earlier studies (in fact the subsequent analysis shows that it was slightly high and further ensembles are now being made with a lower value). The dynamical u and d quarks take a range of masses down as low as a sixth of the (real) m_s . The sets of ensembles divide into two different values of the lattice spacing, 0.13fm and 0.09fm, and the spatial lattice volume is $(2.5\text{fm})^3$, reasonably large. Analysis of hadronic quantities on these ensembles has been done by the MILC and HPQCD collaborations [2].

There are 5 bare parameters of QCD relevant to this analysis: $\alpha_s, m_{u/d}, m_s, m_c$ and m_b . The lattice spacing takes the place of α_s in lattice QCD. It is important that these parameters are fixed using the masses of ‘gold-plated’ hadrons, i.e. hadrons which are

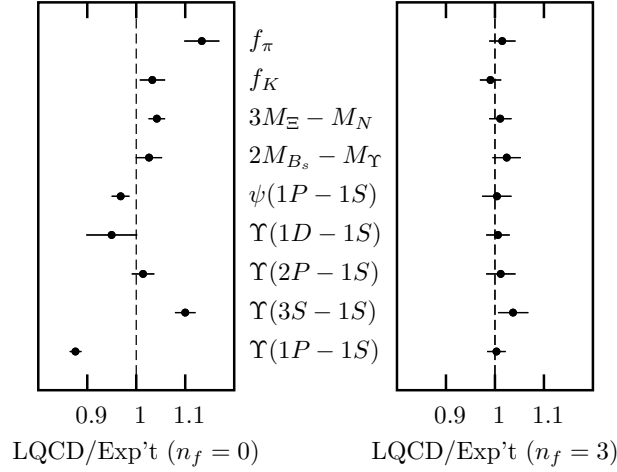


FIGURE 2. Lattice QCD results divided by experiment for a range of ‘gold-plated’ quantities which cover the full range of hadronic physics [2]. The unquenched calculations on the right show agreement with experiment across the board, whereas the quenched approximation on the left give systematic errors of $\mathcal{O}(10\text{-}20\%)$.

well below their strong decay thresholds. Such hadrons are well-defined experimentally and theoretically and should be accurately calculable in lattice QCD. Using them to fix parameters will not then introduce unnecessary additional systematic errors into lattice results for other quantities. This has not always been done in past lattice calculations, particularly in the quenched approximation. It becomes an important issue when lattice QCD is to be used as a precision calculational tool. We use the radial excitation energy in the Y system (i.e. the mass splitting between the Y' and the Y) to fix the lattice spacing and m_π , m_K , m_{D_s} and m_Y to fix the quark masses.

We can then focus on the calculation of other gold-plated masses and decay constants. If QCD is correct and lattice QCD is to work it must reproduce the experimental results for these quantities precisely. Figure 2 shows that this indeed works for the unquenched calculations with u, d and s quarks in the vacuum. A range of gold-plated hadrons are chosen which range from decay constants for light hadrons through heavy-light masses to heavyonium. This tests QCD in different regimes in which the sources of systematic error are very different and stresses the point that QCD predicts a huge range of physics with a small set of parameters.

References [7, 8, 9, 10] give more details on the quantities shown in Figure 2. Here we will discuss some of these. Figure 3 shows the radial and orbital splittings in the $b\bar{b}$ (Y) system for the quenched approximation ($n_f = 0$) and with the dynamical MILC configurations with 3 flavours of dynamical quarks. Our physical understanding of the Y system is very good and there are a lot of gold-plated states well below decay thresholds, which makes it a valuable system for lattice QCD tests. We use the standard lattice NRQCD effective theory for the valence b quarks, which takes advantage of the non-relativistic nature of the bound states. The lattice NRQCD action is accurate through v^4 where v is the velocity of the b quark in its bound state. This means that spin-independent splittings, such as radial and orbital excitations, are simulated through next-to-leading-

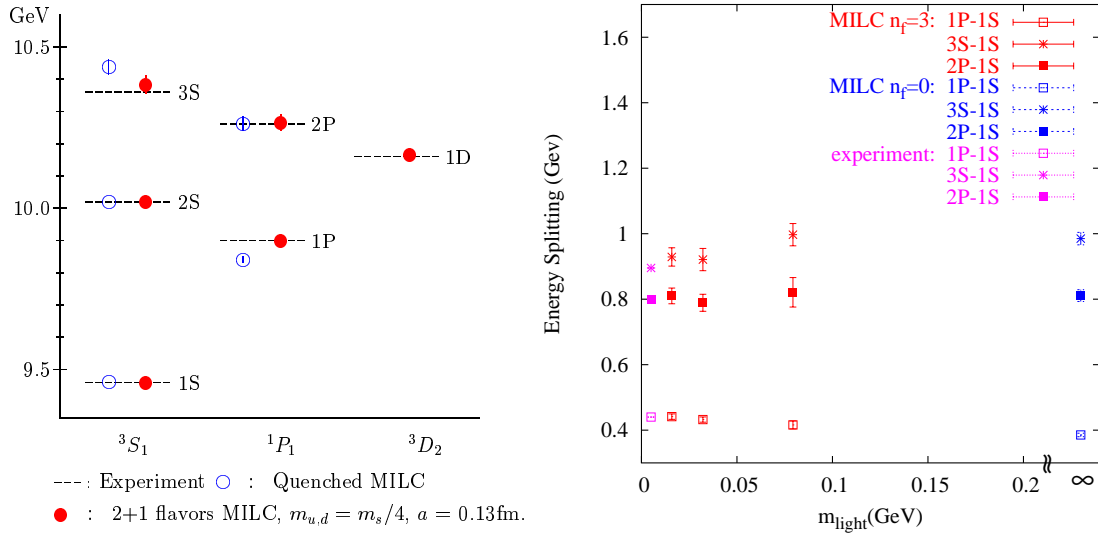


FIGURE 3. Radial and orbital splittings in the Υ system from lattice QCD in the quenched approximation and including u, d and s dynamical quarks. In this plot the lattice spacing was fixed from the radial excitation energy i.e. the splitting between the Υ' and the Υ and the b quark mass was tuned to get the Υ mass correct. The right hand plot shows these splittings plotted as a function of the bare dynamical u/d quark mass for several ensembles of MILC configurations. The leftmost lattice points are the ones used in the left-hand plot and Figure 2.

order and should be accurate to $\approx 1\%$. Thus the test of QCD using these splittings is a very accurate one. The fine structure in the spectrum is only correct through leading-order at present and more work must be done to bring this to the same level and allow tests against, for example, the splittings between the different χ_b states [8].

The Υ system is a good one for looking at the effects of dynamical quarks because we do not expect it to be very sensitive to dynamical quark masses. The momentum transfer inside an Υ is larger than any of the u, d or s masses and so we expect the radial and orbital splittings to simply ‘count’ the number of dynamical quarks once we have reasonably light dynamical quark masses. The righthand plot of Figure 3 shows this to be true - the splittings are independent of the dynamical u/d quark mass in the region we are working in (and therefore for the points plotted in the left hand figure of Figure 3 and in Figure 2).

The π and K decay constants are important light hadron matrix elements, related to the purely leptonic decay rate via a W , and experimentally well-known. These are very sensitive to light quark masses and require a well-controlled extrapolation in the u/d quark mass and interpolation in the s quark mass to get accurate results to compare to experiment. Chiral perturbation theory can be used to perform the u/d quark mass extrapolation provided the masses used on the lattice are small enough for the expansion in powers of quark mass ($\equiv m_\pi^2/(1\text{GeV}^2)$) and its logarithms to work well. In practise this means that second order chiral perturbation theory should work at the 2% level for $m_{u/d} < m_s/2$. Note that the error is set by the largest quark mass used in the chiral fits, *not* the smallest.

Figure 4 shows the results and chiral extrapolation for the decay constants on the

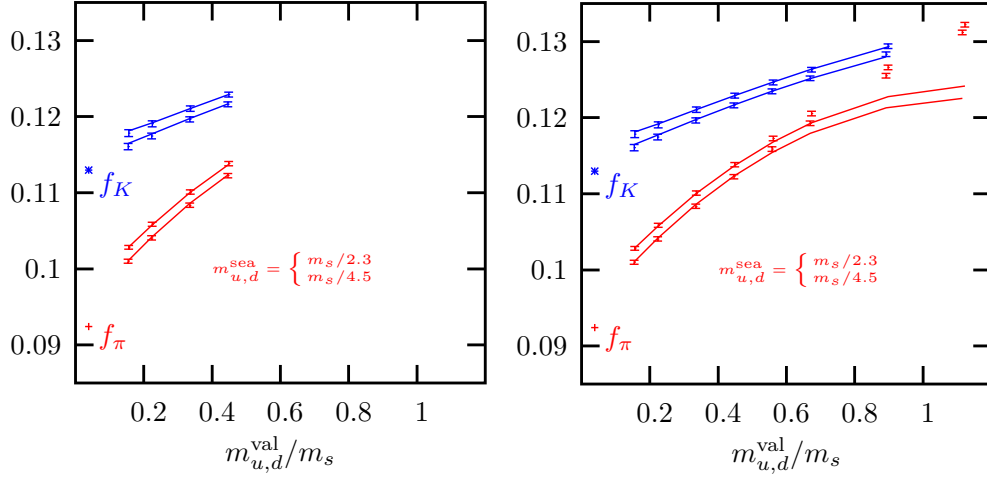


FIGURE 4. Results for the π and K decay constants as a function of light quark mass for two dynamical MILC ensembles at a lattice spacing of 0.09 fm. The plot on the left shows the chiral extrapolation using only results with valence u/d quark masses $< m_s/2$ [2]. The chiral extrapolation must subsequently be corrected for the incorrect valence and sea s quark mass to give the results in Figure 2. The plot on the right shows that this chiral fit from light u/d quark masses does not agree well with the data for $m_{u/d} > m_s/2$.

ensembles of MILC configurations with $m_{u/d}^{sea} = m_s/2.3$ and $m_s/4.5$ at a lattice spacing of 0.09 fm. The curves in the left plot show the chiral extrapolation using only results with $m_{u/d}^{valence} < m_s/2$. This extrapolation has to be corrected, using the lattice results, to interpolate to the physical s quark mass for both sea and valence s quarks. This then gives the results shown in Figure 2 which agree with experiment. The plot on the right shows what happens when the chiral extrapolation fit obtained in the left plot is evaluated for larger valence $m_{u/d}$. The f_π results start to show clear disagreement for $m_{u/d} > m_s/2$, which makes the problem of performing accurate chiral extrapolations using results with $m_{u/d} > m_s/2$ obvious. Previous lattice calculations have been forced by computing cost to work only in this regime, with the added problem that the sea $m_{u/d}$ is also large [11].

Another gold-plated hadron mass is that of the nucleon. A full chiral extrapolation of results for this on the MILC configurations has not yet been done. The left-hand plot of Figure 5 shows very encouraging signs that an answer in agreement with experiment will be found [7]. There is a clear sign of dependence on the lattice spacing, however, which will have to be taken into account. Combinations of baryon masses can be made which are relatively insensitive to u/d quark masses and other effects and it is one of these, $3m_\Xi - m_N$, which is plotted in Figure 2.

It is important to realise that accurate lattice QCD results are not going to be obtainable in the near future for every hadronic quantity of interest. What these results show is that ‘gold-plated’ quantities should now work. Gold-plated hadrons are those well below decay threshold for strong decays. Unstable hadrons, or even those within 100 MeV or so of Zweig-allowed decay modes, have a strong coupling to their real or virtual decay channel which is not correctly simulated on the lattice. The problem is that, with the lattice volumes being used, the allowed non-zero momenta are typically greater

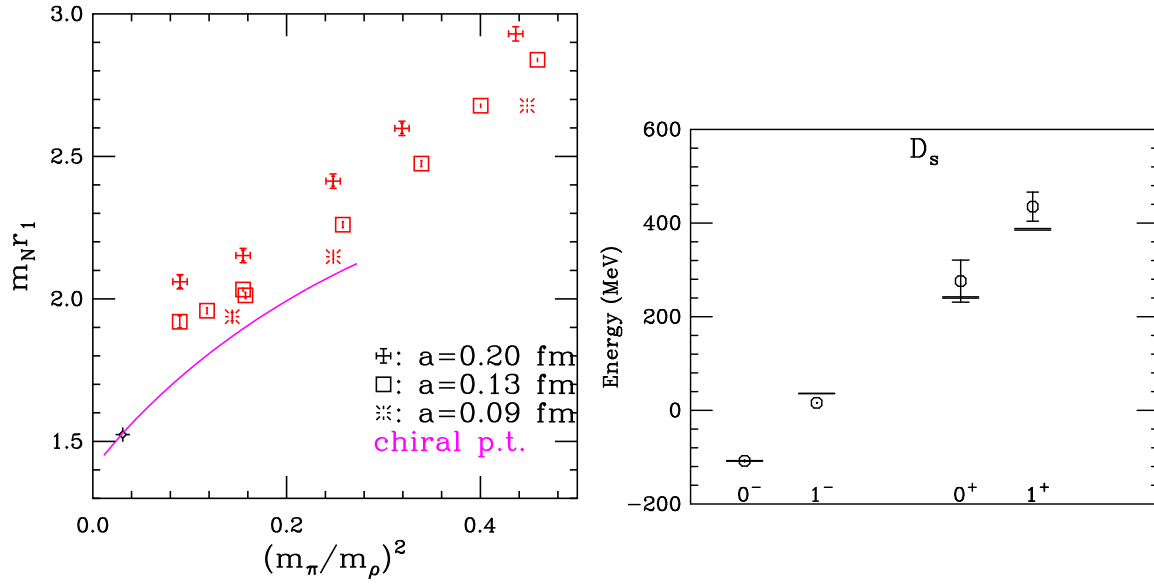


FIGURE 5. The left-hand plot shows results for the nucleon mass on MILC ensembles for different lattice spacings and dynamical quark masses. The nucleon mass is given in units of r_1 , a parameter from the heavy quark potential whose physical value is 0.32fm. The dynamical quark mass is indicated by the variable m_π^2/m_ρ^2 . The curve roughly indicates chiral perturbation theory [7]. The right-hand plot shows the spectrum of D_s states obtained from the MILC dynamical configurations with $m_{u/d} = m_s/4$ and lattice spacing 0.13fm [12].

than 400 MeV and this significantly distorts the decay channel contribution. Much larger simulations will be necessary to handle these hadrons.

Gold-plated hadrons include: π , K , D , D_s , J/ψ , Υ , B , B_s , p , n , Λ , Ω etc. The following are *not* gold-plated: ρ , ϕ , D^* , D_{sJ} , Δ , N^* , pentaquarks, glueballs and hybrids in general. Lattice calculations will not get the masses right for non-gold-plated hadrons even when light dynamical quarks are included. This does not preclude lattice calculations giving useful qualitative results and insight but these points should be borne in mind for any quantitative comparison.

Figure 5 also shows the spectrum of D_s states obtained on the dynamical MILC configurations [12]. The valence c quarks are simulated using an effective theory which, in a similar way to the Υ above, should be accurate for spin-independent splittings and not quite so accurate for fine structure in the spectrum. The hyperfine splitting between the D_s and D_s^* , for example is currently missing a radiative correction to the term in the action proportional to the spin coupling to the chromo-magnetic field. This is being calculated in lattice perturbation theory [3]. Also shown are the scalar and axial vector orbital excitations compared to the recent experimental results for these mesons. The lattice calculation is giving a high result, albeit with large statistical errors at present. However, a high result is consistent with the fact that these mesons are not gold-plated and the lattice calculation does not currently include correctly the coupling to their decay modes.

Decay rates which can be accurately calculated for gold-plated hadrons are those in which there is at most one (gold-plated) hadron in the final state. This therefore includes

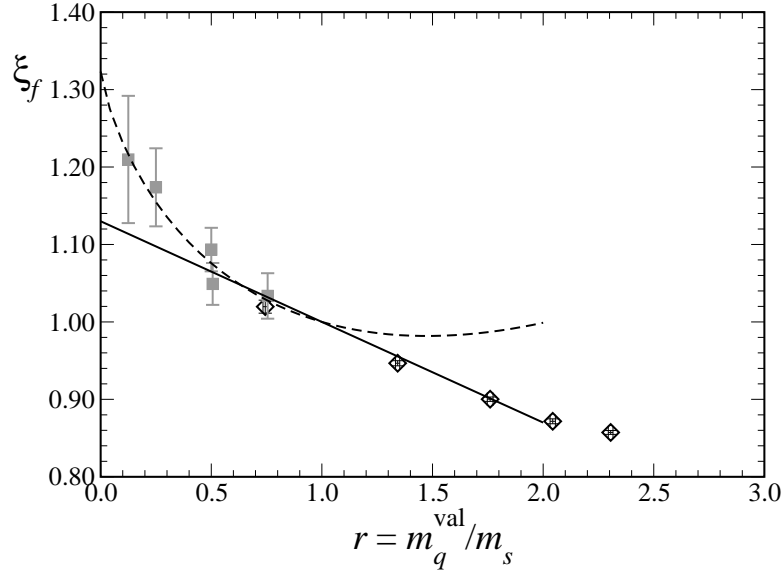


FIGURE 6. Results for the ratio of f_{B_s}/f_{B_d} , as a function of valence u/d quark mass in units of m_s [14]. The grey squares are from the dynamical MILC ensembles including u, d and s dynamical quarks [13]. The black diamonds are from the previous best calculation which included 2 flavours of dynamical quarks with masses $> m_s/2$ [11]. The straight line is a linear extrapolation for the 2 flavour results, the curve includes the possibility of logarithms from chiral perturbation theory. This ratio, for physical u/d masses, appears in the ratio of oscillation frequencies for B_s and B_d mesons, which it is hoped to measure experimentally.

leptonic and semi-leptonic decays and the mixing of neutral B and K mesons. Luckily there is a gold-plated decay mode available to extract each element (except V_{tb}) of the CKM matrix which mixes quark flavours under the weak interactions in the Standard Model:

$$\begin{pmatrix} \mathbf{V}_{ud} & \mathbf{V}_{us} & \mathbf{V}_{ub} \\ \pi \rightarrow l\nu & K \rightarrow l\nu & B \rightarrow \pi l\nu \\ & K \rightarrow \pi l\nu & \\ \mathbf{V}_{cd} & \mathbf{V}_{cs} & \mathbf{V}_{cb} \\ D \rightarrow l\nu & D_s \rightarrow l\nu & B \rightarrow D l\nu \\ D \rightarrow \pi l\nu & D \rightarrow K l\nu & \\ \mathbf{V}_{td} & \mathbf{V}_{ts} & \mathbf{V}_{tb} \\ \langle B_d | \bar{B}_d \rangle & \langle B_s | \bar{B}_s \rangle & \end{pmatrix}$$

As described earlier, the determination of the CKM elements and tests of the self-consistency of the CKM matrix are the current focus for the search for Beyond the Standard Model physics and lattice calculations of these decay rates will be a key factor in the precision with which this can be done.

First calculations on the dynamical MILC configurations have concentrated on the B and B_s leptonic decay rates [13, 12], because these are simplest. They are parameterised by the decay constants, f_B and f_{B_s} , and these are an important component of the mixing rate for these mesons, which constrains V_{ts} and V_{td} . Again one issue in extracting reliable lattice results for f_B and f_{B_s} is the chiral extrapolation in the u/d quark mass. Figure 6 shows results on the MILC configurations for the ratio of f_{B_s}/f_{B_d} plotted against the

valence u/d quark mass [14]. The data extend into the region $m_{u/d} < m_s/2$ which will allow an accurate chiral extrapolation for the first time. Although the statistical errors are currently rather large, it seems likely that the result for this ratio will be larger than previous estimates based on extrapolations from larger u/d masses, and including only two flavours of dynamical quarks [11]. Further calculations of gold-plated matrix elements are in progress [15].

CONCLUSIONS

The impact of lattice QCD calculations has been hindered by the difficulty of including a realistic QCD vacuum. This has led to a level of systematic error far greater than the few percent needed to provide input to tests of the Standard Model, particularly those testing the CKM matrix at B factories. New results this year look set to herald a brighter future in which accurate calculations, at least for gold-plated quantities, are available from the lattice at last.

ACKNOWLEDGMENTS

We are grateful to PPARC, NSF, DoE and the EU for funding this work, and to all our collaborators on [2] for many useful discussions. A version of this talk was also presented at the 2003 Lepton Photon Conference and is published in the proceedings of that meeting.

REFERENCES

1. A. Höcker, H. Lacker, S. Laplace, F. Le Diberder, Eur. Phys. J. C**21** (2001) 225, hep-ph/0104062, <http://www.slac.stanford.edu/~laplace/ckmfitter.html>.
2. C. Davies *et al*, MILC/HPQCD/FNAL/UKQCD collaborations, hep-lat/0304004.
3. H. Trotter, Proceedings of LAT03, hep-lat/0310044.
4. G. P. Lepage, Phys. Rev. D**59**, 074502 (1999), hep-lat/9809157.
5. K. Orginos, D. Toussaint and R. L. Sugar, Phys. Rev. D**60**, 054503 (1999), hep-lat/9903032.
6. C. Bernard *et al*, Phys. Rev. D**64**, 054506 (2001), hep-lat/0104002.
7. S. Gottlieb, Proceedings of LAT03, hep-lat/0310041.
8. A. Gray *et al*, Nucl. Phys. B (Proc. Suppl. **119**), 592 (2003), hep-lat/0209022; C. Davies *et al*, *ibid* 595, hep-lat/0209122.
9. M. di Pierro *et al*, Proceedings of LAT03, hep-lat/0310042.
10. C. Aubin *et al*, Proceedings of LAT03, hep-lat/0309088.
11. S. Aoki *et al*, hep-ph/0307039.
12. M. di Pierro *et al*, Proceedings of LAT03, hep-lat/0310045.
13. M. Wingate, Proceedings of LAT03, hep-lat/0309092.
14. A. Kronfeld, Proceedings of LAT03.
15. J. Shigemitsu *et al*, Proceedings of LAT03, hep-lat/0309039; M. Okamoto *et al*, Proceedings of LAT03, hep-lat/0309107.